

10/660, 556

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NEWS EXPRESS OCTOBER 29 CURRENT WINDOWS VERSION IS V7.01A, CURRENT  
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AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004  
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FILE 'HOME' ENTERED AT 08:10:54 ON 23 NOV 2004

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STRUCTURE FILE UPDATES: 21 NOV 2004 HIGHEST RN 785750-23-4  
DICTIONARY FILE UPDATES: 21 NOV 2004 HIGHEST RN 785750-23-4

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when  
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Crossover limits have been increased. See HELP CROSSOVER for details.

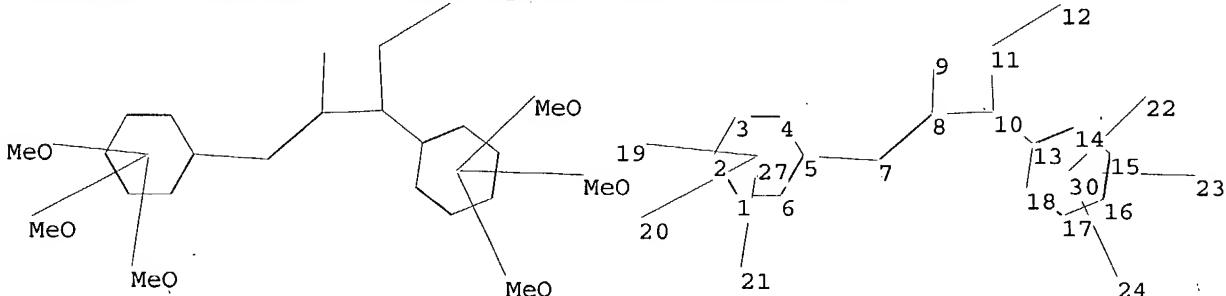
Experimental and calculated property data are now available. For more  
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=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END) :end

=>  
Uploading C:\Program Files\Stnexp\Queries\10660556c.str



chain nodes :

7 8 9 10 11 12 19 20 21 22 23 24

ring nodes :

1 2 3 4 5 6 13 14 15 16 17 18

chain bonds :

5-7 7-8 8-9 8-10 10-11 10-13 11-12

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18

exact bonds :

5-7 7-8 8-9 8-10 10-11 10-13 11-12

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18

isolated ring systems :

containing 1 : 13 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS  
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS  
28:CLASS 29:CLASS 30:CLASS

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L1 STRUCTURE UPLOADED

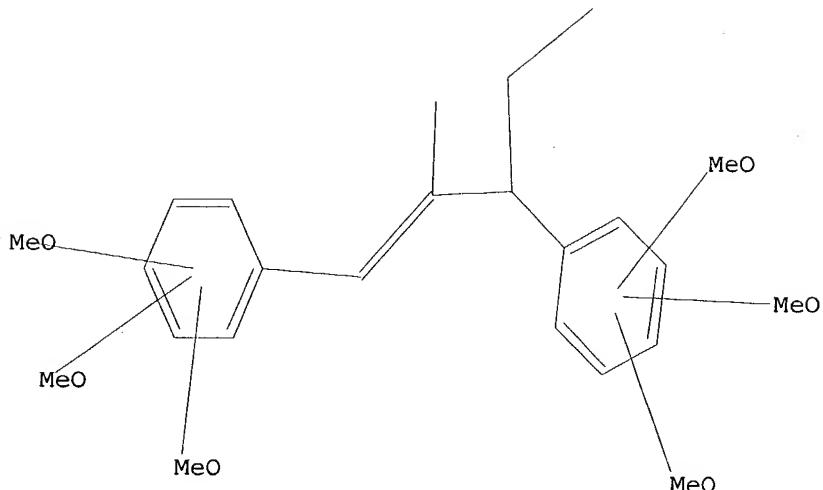
=> que L1

L2 QUE L1

=> d

L2 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.  
L2 QUE L1

=> s 12

SAMPLE SEARCH INITIATED 08:11:36 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 140 TO ITERATE

100.0% PROCESSED 140 ITERATIONS  
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 2091 TO 3509  
PROJECTED ANSWERS: 0 TO 0

L3 0 SEA SSS SAM L1

=> s 12 ful  
FULL SEARCH INITIATED 08:11:43 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 3331 TO ITERATE

100.0% PROCESSED 3331 ITERATIONS  
SEARCH TIME: 00.00.01

2 ANSWERS

L4 2 SEA SSS FUL L1

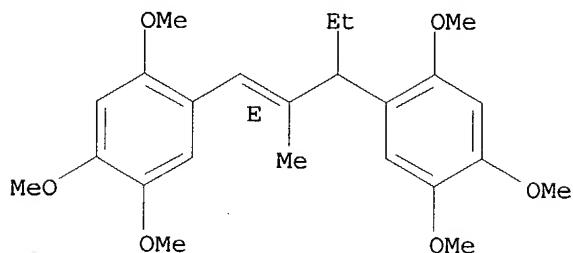
=> d scan

L4 2 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN Benzene, 1,1'-(1E)-3-ethyl-2-methyl-1-propene-1,3-diyl]bis[2,4,5-

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trimethoxy- (9CI)  
MF C24 H32 O6

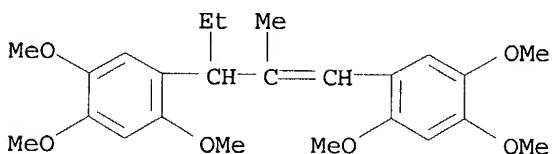
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L4 2 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN Benzene, 1,1'-(3-ethyl-2-methyl-1-propene-1,3-diyl)bis[2,4,5-trimethoxy- (9CI)  
MF C24 H32 O6

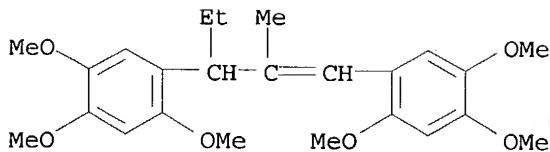


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> d 1-2

L4 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 156246-57-0 REGISTRY  
CN Benzene, 1,1'-(3-ethyl-2-methyl-1-propene-1,3-diyl)bis[2,4,5-trimethoxy- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C24 H32 O6  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT  
DT.CA CAplus document type: Journal; Patent  
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)  
RL.NP Roles from non-patents: FORM (Formation, nonpreparative); PREP (Preparation)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 80423-94-5 REGISTRY

CN Benzene, 1,1'-(1E)-3-ethyl-2-methyl-1-propene-1,3-diyl]bis[2,4,5-trimethoxy- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Benzene, 1,1'-(3-ethyl-2-methyl-1-propene-1,3-diyl)bis[2,4,5-trimethoxy-, (E)-

OTHER NAMES:

CN Diasarone 1

CN NEOLASA-I

FS STEREOSEARCH

DR 130766-51-7, 82373-98-6

MF C24 H32 O6

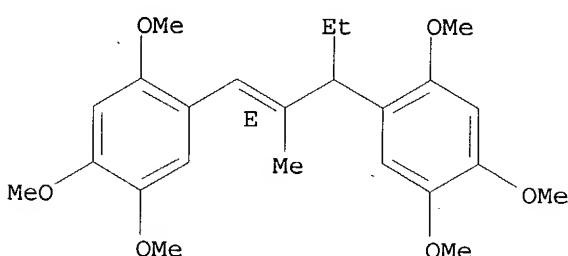
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, NAPRALERT, USPATFULL  
 (\*File contains numerically searchable property data)

DT.CA Cplus document type: Journal; Patent

RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

RL.NP Roles from non-patents: FORM (Formation, nonpreparative); PREP (Preparation); PRP (Properties); RACT (Reactant or reagent)

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

5 REFERENCES IN FILE CA (1907 TO DATE)  
 5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file ca caplus  
 COST IN U.S. DOLLARS  
 FULL ESTIMATED COST

SINCE FILE ENTRY	TOTAL SESSION
159.80	160.01

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=> s 14  
L5 14 L4

=> dup rem 15  
PROCESSING COMPLETED FOR L5  
L6 7 DUP REM L5 (7 DUPLICATES REMOVED)

=> d 1-7 bib ab

L6 ANSWER 1 OF 7 CA COPYRIGHT 2004 ACS on STN DUPLICATE 1  
AN 139:292100 CA

TI Formation of neolignan by DDQ mediated dimerization of dihydroasarone  
IN Sinha, Arun Kumar; Joshi, Bhupendra Prasad; Acharya, Ruchi  
PA Council of Scientific and Industrial Research, India

SO PCT Int. Appl., 37 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003080551	A1	20031002	WO 2002-IN73	20020327
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRAI WO 2002-IN73 20020327

OS CASREACT 139:292100

AB The present invention relates to a novel neolignan 3-ethyl-2-methyl-3-(2'',4'',5''-trimethoxyphenyl)-1-(2',4',5'-trimethoxyphenyl)-1-propene and a process for the preparation of high purity, high yield neolignan,  $\alpha$ -asarone, and 2,4,5-trimethoxyphenylpropionone from  $\beta$ -asarone or  $\beta$ -asarone rich Acorus calamus oil containing  $\alpha$ - and  $\gamma$ -asarone by hydrogenating and dimerizing by treatment with DDQ in presence of an organic acid.

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 7 CA COPYRIGHT 2004 ACS on STN DUPLICATE 2

AN 139:292099 CA

TI DDQ-mediated one step dimerization of  $\beta$ -asarone or  $\beta$ -asarone rich Acorus calamus oil in the formation of novel neolignan  
IN Sinha, Arun Kumar; Joshi, Bhupendra Prasad; Acharya, Ruchi

PA Council of Scientific & Industrial Research, India

SO U.S. Pat. Appl. Publ., 20 pp.

CODEN: USXXCO

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2003187306	A1	20031002	US 2002-108269	20020328
	US 2004049085	A1	20040311	US 2003-660556	20030912
PRAI	US 2002-108269	B3	20020328		
OS	CASREACT 139:292099				
AB	The present invention relates to a novel neolignan, 3-ethyl-2-methyl-3-(2',4',5'-trimethoxyphenyl)-1-(2',4',5'-trimethoxyphenyl)-1-(2',4',5'-trimethoxy)phenyl-1-propene [NEOLASA-I (I)], and a process for the preparation of high purity, higher yield neolignan, $\alpha$ -asarone, 2,4,5-trimethoxy-phenylpropionone from $\beta$ -asarone (II) or $\beta$ -asarone rich Acorus calamus oil containing $\alpha$ - and $\gamma$ -asarone by hydrogenating and dimerizing by treatment with DDQ in presence of an organic acid.				
L6	ANSWER 3 OF 7	CA	COPYRIGHT 2004 ACS on STN		DUPLICATE 3
AN	121:82863	CA			
TI	Chemical structure of 1,3-bis(2,4,5-trimethoxy)phenyl-2-methyl-pentene-1				
AU	Liu, Buming; Ye, Chao; Jiang, Weiheng				
CS	Guangxi Inst. Traditional Med. Pharm., Nanning, 530022, Peop. Rep. China				
SO	Fenxi Huaxue (1994), 22(4), 355-8				
	CODEN: FHHHDT; ISSN: 0253-3820				
DT	Journal				
LA	Chinese				
AB	A new compound of lignans separated from the mother liquor of recrystn. in industrial synthesis of $\alpha$ -asaricin was reported. The structure of the compound was determined by UV, IR, 1H-NMR, 13C-NMR and MS, and revealed to be				
	1,3-bis(2,4,5-trimethoxy)phenyl-2-methyl-1-pentene (I). The compound was synthesized by photochem. reaction using the above mentioned mother liquor. A possible reaction mechanism was also discussed.				
L6	ANSWER 4 OF 7	CA	COPYRIGHT 2004 ACS on STN		DUPLICATE 4
AN	115:278048	CA			
TI	Light-induced transformation of asarone				
AU	Lander, V.; Schreier, P.				
CS	Univ. Wuerzburg, Wuerzburg, D-8700, Germany				
SO	Flavour and Frágrance Journal (1991), 6(1), 21-8				
	CODEN: FFJOED; ISSN: 0882-5734				
DT	Journal				
LA	English				
AB	The stability of $\alpha$ - (I) and $\beta$ -asarone (II) in ethanolic solns. was studied under daylight conditions over a period of 6 mo. After rapid initial light-induced isomerization of I to II, a number of oxidation products, i.e. 2,4,5-trimethoxybenzaldehyde, 1-(2,4,5-trimethoxyphenyl) propan-2-one, and 2,4,5-trimethoxypropiophenone and addition products, i.e. 1-ethoxy-1-(2,4,5-trimethoxyphenyl)propane, (1R,2R; 1S,2S)-1-ethoxy-1-(2,4,5-trimethoxyphenyl)propan-2-ol, (1R,2S; 1S,2R)-1-ethoxy-1-(2,4,5-trimethoxyphenyl)propan-1,2-diol, and (1R,2S; 1S,2R)-1-(2,4,5-trimethoxyphenyl)propan-1,2-diol, as well as the dimers 1-(2',4',5'-trimethoxyphenyl)-2-methyl-3-(2,4,5-trimethoxyphenyl)-1E-pentene (III) and 1-(2',4',5'-trimethoxyphenyl)-2-methyl-3-ethyl-1 $\alpha$ ,2 $\beta$ ,3 $\alpha$ (II)-4,6,7-trimethoxyindane (IV) were detected after extractive sample preparation. In addition, 3 dimers, 1-(2',4',5'-trimethoxyphenyl)-2-methyl-3-(2,4,5-trimethoxyphenyl)-penta-1E,4-diene, 1-(2',4',5'-trimethoxyphenyl)-2-(2,4,5-trimethoxyphenyl)-3,4-dimethylcyclobutane, and 1-(2',4',5'-trimethoxyphenyl)-2-methyl-3-(2,4,5-trimethoxyphenyl)prop-1-en-3-one were tentatively identified. Identification was carried out by capillary gas chromatog. (HRGC) and online HRGC techniques, i.e. HRGC mass spectrometry and HRGC-Fourier transform IR spectroscopy as well as 1H-NMR spectroscopy.				

L6 ANSWER 5 OF 7 CA COPYRIGHT 2004 ACS on STN DUPLICATE 5  
 AN 113:241942 CA  
 TI Structure of (E)-2-methyl-1,3-bis(2,4,5-trimethoxyphenyl)-1-pentene and  
 1-(2,4,5-trimethoxyphenyl)-2-methyl-3-ethyl-4,6,7-trimethoxyindan  
 C24H32O6: two asarone dimers  
 AU Lemini, C.; Mandoki, J. J.; Cruz-Almanza, R.; Toscano, R. A.  
 CS Fac. Med., UNAM, Coyoacan, 04510, Mex.  
 SO Acta Crystallographica, Section C: Crystal Structure Communications  
 (1990), C46(8), 1542-5  
 CODEN: ACSCEE; ISSN: 0108-2701  
 DT Journal  
 LA English  
 AB (E)-2-Methyl-1,3-bis(2,4,5-trimethoxyphenyl)-1-pentene (I) is monoclinic, space group P21/n, with a 7.082(3), b 11.954(7), c 27.136(17) Å, and β 94.14(4)°; d.(calculated) = 1.21 for Z = 4. Final R = 0.056 and R<sub>w</sub> = 0.063 for 2901 reflections. 1-(2,4,5-Trimethoxyphenyl)-2-methyl-3-ethyl-4,6,7-trimethoxyindan (II) is monoclinic space group P21/a with a 17.281(5), b 7.701(1), c 18.057(6) Å, and β 108.23(2)°; d.(calculated) = 1.21 for Z = 4. Final R = 0.045 and R<sub>w</sub> = 0.061 for 2601 reflections. Atomic coordinates are given. The x-ray structures confirm the structures previously assigned on the basis of chemical and NMR spectral evidence. I is non-planar. In II the 5-membered ring adopts an envelope conformation and the substituents at C(1) and C(3) are antiperiplanar to the Me group at C(2). In both isomers the orientation of the trimethoxyphenyl substituent is determined by C-H...O intramol. interactions. The packing in the crystal is entirely due to van der Waals forces.

L6 ANSWER 6 OF 7 CA COPYRIGHT 2004 ACS on STN DUPLICATE 6  
 AN 97:38740 CA  
 TI The active substances of Asarum europeum L. XV. Structure of the  
 diasarones  
 AU Bohlmann, Ferdinand; Gracza, Lajos  
 CS Inst. Org. Chem., Tech. Univ. Berlin, Berlin, D 1000, Fed. Rep. Ger.  
 SO Archiv der Pharmazie (Weinheim, Germany) (1982), 315(5), 474-6  
 CODEN: ARPMAZ; ISSN: 0365-6233 RSI.A7  
 DT Journal  
 LA German  
 AB Diasarone, prepared by the method of T. Szeki (1906), consists of 2 substances, diasarone-1 (I) and diasarone-2 (II).  
 L6 ANSWER 7 OF 7 CA COPYRIGHT 2004 ACS on STN DUPLICATE 7  
 AN 96:34762 CA  
 TI Synthesis of a novel asarone dimer  
 AU Lemini, C.; Cruz, R.; Sanchez, I. H.  
 CS Fac. Med., Univ. Nac. Auton. Mexico, Mexico City, Mex.  
 SO Organic Preparations and Procedures International (1981), 13(5), 374-8  
 CODEN: OPPIAK; ISSN: 0030-4948  
 DT Journal  
 LA English  
 AB Title compds. I and II were prepared as anticholesteremics (no data). Thus, asarone was treated at room temperature with PBr<sub>3</sub> for 3 h to give 87% E-I. Treating I with PBr<sub>3</sub> for 24 h gave 78% II. I was converted to II by acid catalysis.

=> log y  
 COST IN U.S. DOLLARS SINCE FILE TOTAL  
 FULL ESTIMATED COST ENTRY SESSION  
 20.80 180.81  
 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL

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ENTRY	SESSION
-4.62	-4.62

STN INTERNATIONAL LOGOFF AT 08:18:04 ON 23 NOV 2004